Title	**REBEL (REdox state role in Bio-inspired ELementary reactions)**
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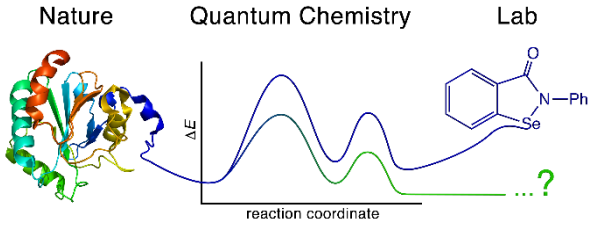
Project description:

Computational methodologies are nowadays well consolidated in a multi-scale range, so that accurate *in silico experiments* can be carried out on molecules with tenths of atoms as well as on very large systems like biomolecules. An ambitious goal in computational chemistry is the design of functional molecules, i.e. drugs, devices, catalysts, and in most cases inspiration is searched in nature. A solid and rigorous approach to the design of bio-inspired molecules, i.e. catalysts, requires investigation of the natural systems as well as a bottom-up approach starting from small model molecules. These studies are intrinsically multi-scale and benefit of data from synthesis and measurements set up by collaborators. Systems of interest are anti-oxidant enzymes, such as GPx and PRx, proteins in which the chemistry of chalcogens (selenium and sulfur) is fundamental. In particular, the REDOX state of the catalytic center seems to play a key-role, still under debate. The mechanisms of oxidation phenomena will be studied in the enzymes as well as in model systems and molecular catalysts/drugs. The PhD student will gain experience with advanced computational methodologies, among which quantum chemistry and molecular dynamics approaches and his research tasks will certainly gain profit of the multiscale skills acquired in the years in the group of Theoretical Chemistry (from molecular level to continuum). In addition, he/she will learn and practice script/programming languages and abilities to work with supercomputers (local and national facilities). Requisites are chemical curiosity, passion for numerical problems and computers and inclination to apply consolidated chemistry background to solve problems.



Publications:

- Ribaudo, G.; Bellanda, M.; Menegazzo, I.; Wolters, L. P.; Bortoli, M.; Ferrer-Sueta, G.; Zagotto, G.; Orian, L. Mechanistic insight into the oxidation of organic phenylselenides by H_2O_2 *Chem. Eur. J.* **2017** *23*, 2405-2422.
- Bortoli, M.; Wolters, L.P.; Orian, L.; Bickelhaupt, F. M. *J. Chem. Th. Comp.* **2016** *12,* 2752-2761.
- Orian, L.; Toppo, S. Organochalcogen peroxidase mimetics as potential drugs: a long story of a promise still unfulfilled *Free Rad. Biol. Med.* **2014** *66,* 65-74

Collaborations/Network:

Theoretical Chemistry Group VU Amsterdam (The Netherlands) (Prof. F.M. Bickelhaupt and Prof. Célia Fonseca Guerra)

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